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High temperature and high pressure gas cell for quantitative spectroscopic measurements

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ABSTRACT

A high temperature and high pressure gas cell (HTPGC) has been manufactured for quantitative spectroscopic measurements in the pressure range 1–200 bar and temperature range 300–1300 K. In the present work the cell was employed at up to 100 bar and 1000 K, and measured absorption coefficients of a CO_2–N_2 mixture at 100 bar and 1000 K are revealed for the first time, exceeding the high temperature and pressure combinations previously reported. This paper discusses the design considerations involved in the construction of the cell and presents validation measurements compared against simulated spectra, as well as published experimental data.

1. Introduction

The interest in high temperature and high pressure CO_2 data emerges from two very different fields of research; the scientific study of the atmosphere of Mars and Venus [1] and the industrially motivated research in combustion engines for which high temperature and pressure absorption spectra are required for proper modeling of the heat transfer processes [2]. This work is motivated by the latter, and has formed part of a larger project named Radiade [3], which focusses on the improvement of radiant heat transfer models at high pressure and temperature for modeling of combustion, fluid flow, and radiation heat transfer phenomena as well as their mutual interactions [4]. However, the experimental results presented in this paper are expected be of equal interest to the first mentioned research area as the most recent release notes of the HITRAN (2012) database states; "*High-quality reference spectroscopic data for the carbon dioxide molecule remains one of the top priorities for the HITRAN database, due in part to its importance for the environmental satellite missions, including OCO-2 and GOSAT and its importance to the studies of the atmospheres of Mars and Venus*" [5].

A number of gas cells have already been constructed and utilized to acquire spectroscopic measurements of CO_2 at elevated temperatures and pressures [6–8]. Common to the gas cells is that they are built of metal, a material which is easy to machine and exhibits good thermal conductivity, assuring uniform temperature distribution. However, metal loses its strength at high temperature. In recent work by Stefani et al. [8] a commercial gas cell was employed which was designed for temperatures up to 650 K and pressures up to 200 bar. In terms of pressure this is sufficient to cover the peak pressures inside two-stroke ship engines, however, combustion temperatures are much higher. Thus for combustion heat transfer modeling, experimental data at even higher temperatures is required. The present gas cell cover the pressure levels

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typical for combustion engines, and raises the temperature to as high as 1300 K. Whilst this offers a great step into unexplored territory, it remains a demand for future gas cells to reach temperatures above 2400 K at high pressures to cover all engine conditions.

The present paper discusses the design of HTPGC including the choices and trade-offs involved. The cell is validated against previously published experiments as well simulations based on the HITRAN2012 database [5]. Finally, a recently recorded spectrum of 5% CO_2 in N_2 at 101 bar and 1000 K is presented, well outside the parametric space of previous experimental gas cell studies of infrared CO_2 absorption.

2. Design of the high temperature and high pressure gas cell

The design of a high temperature and high pressure gas cell involves a number of choices and trade-offs, including cell material, window material, sealing method, dimensioning and safety. A sketch of HTPGC is shown in Fig. 1. A 3-D drawing of the cell is shown at the top and a cross-section including dimensions is shown at the bottom of the figure. The outer and inner tubes of the cell are made of a high grade ceramic (aluminum oxide, 99.5%) that exhibits great strength even at high temperatures where metal capitulates. Ceramics are fragile and difficult to machine but, in return, exhibit low thermal expansion and are less troubled by undesired surface reactions. The ceramic tubes are concentrically aligned as shown in the figure and fixed by two water cooled brass flanges in the ends. The brass flanges are bonded to the ceramic by means of a high temperature epoxy (J–B Weld). Holes located at the center of each flange allow for a straight line of sight through the inner tubes.

Slightly tilted 3.0 mm thick ½″ sapphire windows are glass bonded to each end of the inner tubes in order to obtain a gas tight high temperature seal. The use of sapphire windows restricts the wavelength range that can be studied with this gas cell since sapphire blocks radiation above ~6 μm, depending on window thickness and temperature. On the other hand, sapphire is extremely robust and has a thermal expansion that is well matched to the ceramics in the target temperature range. The latter is crucial in order to reduce thermal stresses. The volume confined by the two sapphire windows and the outer tube is the optically accessible measurement volume with a path length of 30.3 mm ± 0.1 mm. The choice of a relatively short path length is advantageous at high gas densities. The low thermal expansion coefficient implies that the temperature dependence of the path length is very small, e.g. at 1000 K a pathlength increase of 0.02 mm is estimated compared to room temperature. Three separate heating coils protected by ceramic beads are wound around the outer ceramic tube (not shown in the figure). One heating coil is covering the central zone around the measurement volume and the two other heating coils are placed symmetrically at each side next to the central zone. At each zone a thermocouple is placed and temperature control is applied to each zone independently, assuring high temperature uniformity over the measurement path and compensation for additional heat loss at the windows. In addition to the three thermocouples used for controlling the heat zones, a total of six very thin ceramic tubes are running parallel with the center axis in the cavity between the outer and inner ceramic tubes. These tiny tubes are exactly thick enough for a 0.5 mm type N thermocouple to be inserted from the outside, and under steady temperature conditions, the thermocouple reflects the gas temperature. A calibrated thermocouple can be cautiously slided inside the ceramic tube to map the internal temperature field over the measurement path. Although the thermocouple is calibrated to a specified accuracy of 0.4 K at 300 K and 0.8 K at 1000 K, the uncertainty of the measured gas temperature is larger because it is dominated by temperature distributions, which is discussed in Section 3.1.

The heating zones are thermally insulated in order to reduce energy losses. A picture of the insulated gas cell is shown in Fig. 2. One of the end flanges can be seen to the left along with a small piece of the outer ceramic tube.

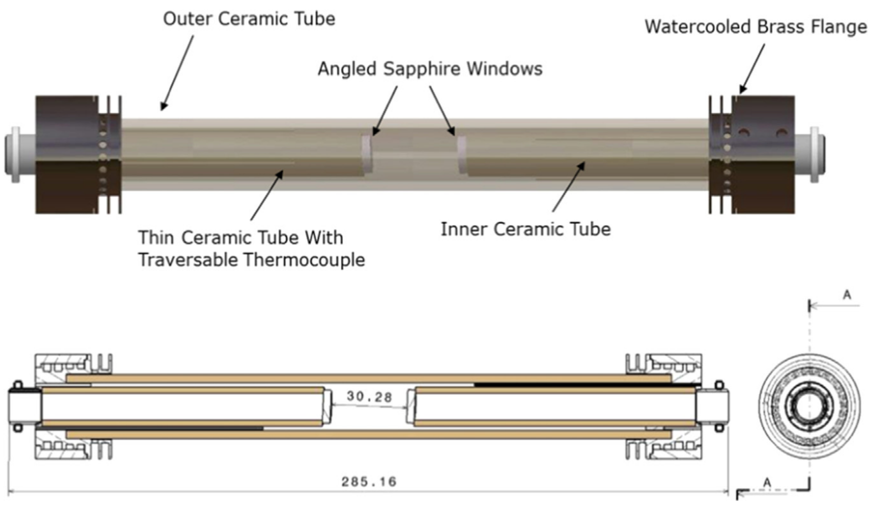

Fig. 1. Top: 3-D drawing of HTPGC. Bottom: cross-section sketch of HPTGC including dimensions in mm. The ends of the inner ceramic tubes at the flanges are open.